

Fumaric acid, 2,4,4-trimethylpentyl hept-2-yl ester

Inchi:	InChI=1S/C19H34O4/c1-7-8-9-10-16(3)23-18(21)12-11-17(20)22-14-15(2)13-19(4,5)6/h1
InchiKey:	KKIANBFWNYWUBX-VAWYXSNFSA-N
Formula:	C19H34O4
SMILES:	CCCCC(C)OC(=O)C=CC(=O)OCC(C)CC(C)(C)C
Mol. weight [g/mol]:	326.47

Physical Properties

Property code	Value	Unit	Source
gf	-280.56	kJ/mol	Joback Method
hf	-827.18	kJ/mol	Joback Method
hfus	36.28	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.670		Crippen Method
mvol	289.150	ml/mol	McGowan Method
pc	1219.99	kPa	Joback Method
rinpol	2047.00		NIST Webbook
rinpol	2047.00		NIST Webbook
tb	786.75	K	Joback Method
tc	977.58	K	Joback Method
tf	415.55	K	Joback Method
vc	1.105	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.41	J/molxK	786.75	Joback Method
cpg	904.09	J/molxK	818.55	Joback Method
cpg	920.76	J/molxK	850.36	Joback Method
cpg	936.43	J/molxK	882.16	Joback Method
cpg	951.16	J/molxK	913.97	Joback Method
cpg	964.98	J/molxK	945.77	Joback Method
cpg	977.93	J/molxK	977.58	Joback Method
dvisc	0.0012707	Paxs	415.55	Joback Method

dvisc	0.0004790	Paxs	477.42	Joback Method
dvisc	0.0002259	Paxs	539.28	Joback Method
dvisc	0.0001243	Paxs	601.15	Joback Method
dvisc	0.0000765	Paxs	663.02	Joback Method
dvisc	0.0000511	Paxs	724.88	Joback Method
dvisc	0.0000364	Paxs	786.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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